



ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26  
27 28

ring bonds :

1-2 1-6 1-9 2-3 2-10 3-4 3-12 4-5 4-21 5-6 5-23 6-7 7-8 7-17 8-9 8-20 9-27  
10-11 10-25 11-12 11-13 12-16 13-14 14-15 15-16 17-18 18-19 19-20 21-22 22-23  
24-25 24-28 25-26 26-27 27-28

exact/norm bonds :

1-9 2-10 3-12 4-21 5-23 6-7 8-9 9-27 10-11 10-25 21-22 22-23 24-25 24-28 25-26  
26-27 27-28

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-17 8-20 11-12 11-13 12-16 13-14 14-15 15-16 17-18  
18-19 19-20

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom  
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom